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The largest Hosoya index of $(n, n+1)$-graphs☆

Hanyuan Deng

College of Mathematics and Computer Science, Hunan Normal University, Changsha, Hunan 410081, PR China

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ABSTRACT

The Hosoya index of a graph is defined as the total number of its matchings. In this paper, we obtain that the largest Hosoya index of $(n, n+1)$-graphs is $f(n+1)+f(n-1)+2f(n-3)$, where $f(n)$ is the nth Fibonacci number, and we characterize the extremal graphs.

1. Introduction

The Hosoya index or Z-index $z(G)$ of a graph G is the total number of its matchings plus one; the one corresponds to a matching in a set with zero edges. The Hosoya index is a prominent example of topological indices which are of interest in combinatorial chemistry. It is defined as the total number of matchings (independent edge subsets) of a graph. The Z-index was introduced by Hosoya [1,2] in 1971, and it turned out to be applicable to several questions of molecular chemistry. For example, the connections with physico-chemical properties such as boiling point, entropy or heat of vaporization are well studied.

Several papers deal with the characterization of the extremal graphs with respect to the Hosoya index in several given graph classes. Usually, trees, unicyclic graphs and certain structures involving pentagonal and hexagonal cycles are of major interest [3–12].

In this paper, we deal with the characterization of the extremal graphs with the largest Hosoya index among all $(n, n+1)$-graphs, i.e., the simple connected graphs with n vertices and $n+1$ edges.

Let $G = (V, E)$ be a simple connected graph with the vertex set V and the edge set E. For any $v \in V$, $N_G(v)$ denotes the neighbors of v, and $d_G(v) = |N(v)|$ is the degree of v. A leaf is a vertex of degree one.

If $E' \subseteq E(G)$ and $W \subseteq V(G)$, then $G - E'$ and $G - W$ denote the subgraphs of G obtained by deleting the edges of E' and the vertices of W, respectively. If a graph G has components $G_1, G_2, \ldots, G_t$, then G is denoted by $\bigcup_{i=1}^{t} G_i$. We denote by P_n the path on n vertices and by C_n the cycle on n vertices.

The following basic results will be used.

(i) If v is a vertex of G, then

$$z(G) = z(G - \{v\}) + \sum_{x \in N_G(v)} z(G - \{v, x\}). \tag{1}$$

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E-mail address: hydeng@hunnu.edu.cn.

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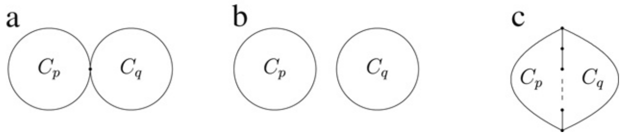

Fig. 1. The subgraphs induced by the cycles of an $(n, n+1)$-graph.

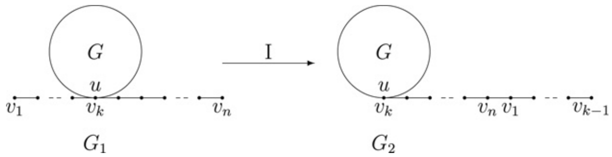

Fig. 2. Transformation 1.

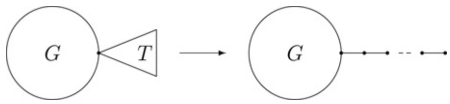

Fig. 3. The graphs in Remark 1.

(ii) If uv is an edge of G, then

$$z(G) = z(G - uv) + z(G - \{u, v\}). \tag{2}$$

(iii) If G is a graph with components $G_1, G_2, \ldots, G_k$, then

$$z(G) = \prod_{i=1}^{k} z(G_i).$$

(vi) $z(C_n) = f(n-1) + f(n+1)$ for $n \geq 3$.
(v) $z(P_0) = 1, z(P_1) = 1$ and $z(P_n) = f(n+1)$ for $n \geq 2$
where $f(0) = 0, f(1) = 1$ and $f(n) = f(n-1) + f(n-2)$ for $n \geq 2$ denotes the sequence of Fibonacci numbers.

The following property of the Fibonacci numbers is very well known and can be seen immediately by plugging into Binet's formula.

Lemma 1.1. *$f(n) = f(k)f(n-k+1) + f(k-1)f(n-k)$ for $1 \leq k \leq n$.*

Let $\mathcal{G}(n, n+1)$ be the set of simple connected graphs with n vertices and $n+1$ edges. For any graph $G \in \mathcal{G}(n, n+1)$, there are two cycles C_p and C_q in G. We divide all the $(n, n+1)$-graphs with two cycles of lengths p and q into three classes.

(1) $\mathcal{A}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have only one common vertex;
(2) $\mathcal{B}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have no common vertex;
(3) $\mathcal{C}(p, q, r)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have a common path of length $r+1$, $r \geq 0$.

Note that the subgraph induced by the cycles of $G \in \mathcal{A}(p, q)$ (or $\mathcal{B}(p, q)$, $\mathcal{C}(p, q, r)$) is shown in Fig. 1(a) (or (b),(c)) and $\mathcal{C}(p, q, r) = \mathcal{C}(p, p+q-2r+2, p-r-2) = \mathcal{C}(p+q-2r-2, q, q-r-2)$.

2. Transformations increasing the Hosoya index

For convenience, we introduce in this section three transformations, which increase the Hosoya index.

Transformation 1. Let $G \neq P_1$ be a connected graph and choose $u \in V(G)$. G_1 denotes the graph that results from identifying u with the vertex v_k of a simple path $v_1 v_2 \cdots v_n$, $1 < k < n$; G_2 is obtained from G_1 by deleting $v_{k-1}v_k$ and adding $v_1 v_n$ (see Fig. 2).

Lemma 2.1 ([9]). *Let G_1 and G_2 be the graphs in Fig. 2. Then $z(G_1) < z(G_2)$.*

Remark 1. Repeating Transformation 1, any tree T of size t attached to a graph G can be changed into a path with t edges as shown in Fig. 3. The Hosoya index increases by this transformation.

Transformation 2. Let $P = uu_1u_2 \cdots u_t v$ be a path in G and $G \neq P$, where the degrees of $u_1, \ldots, u_t$ in G are 2 (such a path P is called an internal path of G). G_1 denotes the graph that results from identifying u with the vertex v_k of a simple path $v_1 v_2 \cdots v_k$ and identifying v with the vertex v_{k+1} of another simple path $v_{k+1}v_{k+2} \cdots v_n$, $1 < k < n-1$; G_2 is obtained from G_1 by deleting $v_{k-1}v_k$ and adding $v_1 v_n$, G_3 is obtained from G_1 by deleting $v_{k+1}v_{k+2}$ and adding $v_1 v_n$ (see Fig. 4).

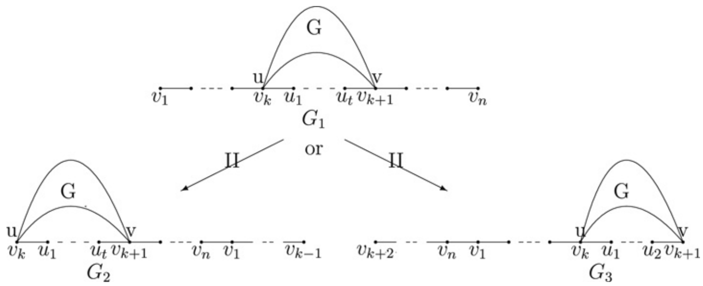

Fig. 4. Transformation 2.

Lemma 2.2. *Let G_1, G_2 and G_3 be the graphs in Fig. 4. Then $z(G_1) < z(G_2)$ or $z(G_1) < z(G_3)$.*

Proof. Let $X = N_G(u) - \{u_1\}$ and $Y = N_G(v) - \{u_t\}$.

$$A = z(G - \{u, u_1, \dots, u_t, v\})$$
$$B = \sum_{y \in Y} z(G - \{u, u_1, \dots, u_t, v, y\})$$
$$C = \sum_{x \in X} z(G - \{u, u_1, \dots, u_t, v, x\})$$
$$D = \sum_{x \in X} \sum_{y \in Y} z(G - \{u, u_1, \dots, u_t, v, x, y\}).$$

By Eq. (1),

$$\begin{aligned}
z(G_1) &= z(G_1 - \{u\}) + \sum_{x \in X} z(G_1 - \{u, x\}) + z(G_1 - \{u, u_1\}) + z(G_1 - \{u, v_{k-1}\}) \\
&= z(G_1 - \{u, v\}) + \sum_{y \in Y} z(G_1 - \{u, v, y\}) + z(G_1 - \{u, v, u_t\}) + z(G_1 - \{u, v, v_{k+2}\}) \\
&\quad + \sum_{x \in X} z(G_1 - \{u, x, v\}) + \sum_{x \in X} \sum_{y \in Y} z(G_1 - \{u, x, v, y\}) + \sum_{x \in X} z(G_1 - \{u, x, v, u_t\}) \\
&\quad + \sum_{x \in X} z(G_1 - \{u, x, v, v_{k+2}\}) + z(G_1 - \{u, u_1, v\}) + \sum_{y \in Y} z(G_1 - \{u, u_1, v, y\}) + z(G_1 - \{u, u_1, v, u_t\}) \\
&\quad + z(G_1 - \{u, u_1, v, v_{k+2}\}) + z(G_1 - \{u, v_{k-1}, v\}) + \sum_{y \in Y} z(G_1 - \{u, v_{k-1}, v, y\}) \\
&\quad + z(G_1 - \{u, v_{k-1}, v, u_t\}) + z(G_1 - \{u, v_{k-1}, v, v_{k+2}\}) \\
&= Af(k)f(n-k)f(t+1) + Bf(k)f(n-k)f(t+1) + Af(k)f(n-k)f(t) \\
&\quad + Af(k)f(n-k-1)f(t+1) + Cf(k)f(n-k)f(t+1) + Df(k)f(n-k)f(t+1) \\
&\quad + Cf(k)f(n-k)f(t) + Cf(k)f(n-k-1)f(t+1) + Af(k)f(n-k)f(t) \\
&\quad + Bf(k)f(n-k)f(t) + Af(k)f(n-k)f(t-1) + Af(k)f(n-k-1)f(t) \\
&\quad + Af(k-1)f(n-k)f(t+1) + Bf(k-1)f(n-k)f(t+1) \\
&\quad + Af(k-1)f(n-k)f(t) + Af(k-1)f(n-k-1)f(t+1) \\
&= A[f(k)f(n-k)f(t+1) + f(k)f(n-k)f(t) + f(k)f(n-k-1)f(t+1) \\
&\quad + f(k)f(n-k)f(t) + f(k)f(n-k)f(t-1) + f(k)f(n-k-1)f(t) \\
&\quad + f(k-1)f(n-k)f(t+1) + f(k-1)f(n-k)f(t) + f(k-1)f(n-k-1)f(t+1)] \\
&\quad + B[f(k)f(n-k)f(t+1) + f(k)f(n-k)f(t) + f(k-1)f(n-k)f(t+1)] \\
&\quad + C[f(k)f(n-k)f(t+1) + f(k)f(n-k)f(t) + f(k)f(n-k-1)f(t+1)] \\
&\quad + Df(k)f(n-k)f(t+1) \\
&= A[f(k+1)f(n-k+1)f(t+1) + f(k+1)f(n-k)f(t) + f(k)f(n-k+1)f(t) \\
&\quad + f(k)f(n-k)f(t-1)] + B[f(k+1)f(n-k)f(t+1) + f(k)f(n-k)f(t)] \\
&\quad + C[f(k)f(n-k+1)f(t+1) + f(k)f(n-k)f(t)] \\
&\quad + Df(k)f(n-k)f(t+1).
\end{aligned}$$

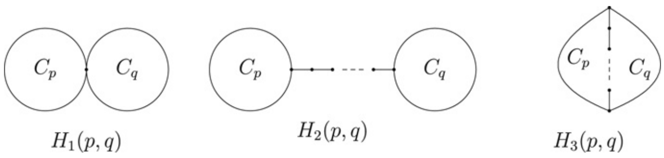

Fig. 5. The graphs $H_i(p, q)$, $i = 1, 2, 3$.

Similarly, we have

$$\begin{aligned} z(G_2) &= A[f(n)f(t+1) + f(n+1)f(t) + f(n-1)f(t-1)] + B[f(n-1)f(t+1) + f(n-1)f(t)] \\ &\quad + C[f(n)f(t+1) + f(n-1)f(t)] + Df(n-1)f(t+1); \\ z(G_3) &= A[f(n)f(t+1) + f(n+1)f(t) + f(n-1)f(t-1)] + B[f(n)f(t+1) + f(n-1)f(t)] \\ &\quad + C[f(n-1)f(t+1) + f(n-1)f(t)] + Df(n-1)f(t+1). \end{aligned}$$

If $B \le C$, then by Lemma 1.1

$$\begin{aligned} \Delta_1 &= z(G_2) - z(G_1) \\ &= A[(f(n) - f(k+1)f(n-k+1))f(t+1) + (f(n+1) - f(k+1)f(n-k) \\ &\quad - f(k)f(n-k+1))f(t) + (f(n-1) - f(k)f(n-k))f(t-1)] \\ &\quad + B[(f(n-1) - f(k+1)f(n-k))f(t+1) + (f(n-1) - f(k)f(n-k))f(t)] \\ &\quad + C[(f(n) - f(k)f(n-k+1))f(t+1) + (f(n-1) - f(k)f(n-k))f(t)] \\ &\quad + D[f(n-1) - f(k)f(n-k)]f(t+1) \\ &= A[-f(k-1)f(n-k-1)f(t+1) + f(k-1)f(n-k-1)f(t) + f(k-1)f(n-k-1)f(t-1)] \\ &\quad + B[-f(k-1)f(n-k-2)f(t+1) + f(k-1)f(n-k-1)f(t)] \\ &\quad + C[f(k-1)f(n-k)f(t+1) + f(k-1)f(n-k-1)f(t)] + Df(k-1)f(n-k-1)f(t+1) \\ &= B[-f(k-1)f(n-k-2)f(t+1) + f(k-1)f(n-k-1)f(t)] \\ &\quad + C[f(k-1)f(n-k)f(t+1) + f(k-1)f(n-k-1)f(t)] + Df(k-1)f(n-k-1)f(t+1) > 0. \end{aligned}$$

If $B > C$, then by Lemma 1.1

$$\begin{aligned} \Delta_2 &= z(G_3) - z(G_1) \\ &= A[(f(n) - f(k+1)f(n-k+1))f(t+1) + (f(n+1) - f(k+1)f(n-k) \\ &\quad - f(k)f(n-k+1))f(t) + (f(n-1) - f(k)f(n-k))f(t-1)] \\ &\quad + B[(f(n) - f(k+1)f(n-k))f(t+1) + (f(n-1) - f(k)f(n-k))f(t)] \\ &\quad + C[(f(n-1) - f(k)f(n-k+1))f(t+1) + (f(n-1) - f(k)f(n-k))f(t)] \\ &\quad + D[f(n-1) - f(k)f(n-k)]f(t+1) \\ &= B[f(k)f(n-k-1)f(t+1) + f(k-1)f(n-k-1)f(t)] \\ &\quad + C[-f(k-2)f(n-k-1)f(t+1) + f(k-1)f(n-k-1)f(t)] + Df(k-1)f(n-k-1)f(t+1) > 0. \end{aligned}$$

The proof is completed. □

Remark 2. If G is the $(n, n+1)$-graph with trees $T_1, \ldots, T_k$ of sizes $t_1, \ldots, t_k$ attached to one of the graphs $H_i(p, q)$ $(i = 1, 2, 3)$ in Fig. 5, then these trees are changed into paths of sizes $t_1, \ldots, t_k$ after repeating Transformation 1. Let us continue repeating Transformation 2, these paths will be combined into one path. So, G can be changed into an $(n, n+1)$-graph with at least one path attached to one of the graphs $H_i(p, q)$, and the Hosoya index increases by these transformations.

The proof of the following lemma is obvious.

Lemma 2.3. (i) *Let $P = v_1v_2\cdots v_n$ be a path of length $n-1$, $n > 1$. $M_1(P)$ is the set of matchings of P containing v_1v_2 and $M_2(P)$ is the set of matchings of P containing v_nv_{n-1}. Define $\xi_P(v_iv_{i+1}) = v_{n-i+1}v_{n-i}$ for $i = 1, 2, \ldots, n-1$. Then ξ_P is a bijective mapping between $M_2(P)$ and $M_1(P)$;*

(ii) *Let $C = v_1v_2\cdots v_nv_{n+1}$ be a cycle of length n, $v_{n+1} = v_1$. $M_1(C)$ is the set of matchings of C containing v_1v_2 and $M_2(C)$ is the set of matchings of P containing v_1v_n. $\xi_C(v_iv_{i+1}) = v_{n-i+2}v_{n-i+1}$ for $i = 1, 2, \ldots, n$. Then ξ_C is a bijective mapping between $M_2(C)$ and $M_1(C)$.*

Transformation 3. Let $P = u_0u_1u_2\cdots u_{t+1}$ be a path or a cycle (if $u_0 = u_{t+1}$) in G, where the degrees of $u_1, \ldots, u_t$ in G are 2, $t \ge 1$. G_1 denotes the graph that results from identifying u_r $(0 \le r \le t)$ with the vertex v_k of a simple path $v_1v_2\cdots v_k$; G_2 is obtained from G_1 by deleting u_ru_{r+1} and adding $u_{r+1}v_1$ (see Fig. 6).

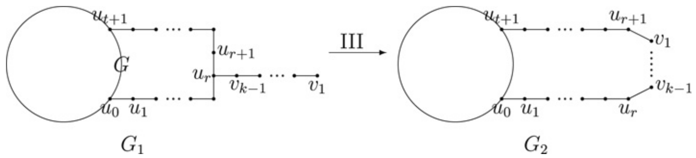

Fig. 6. Transformation 3.

Lemma 2.4. *Let G_1 and G_2 be the graphs in Fig. 6. Then $z(G_1) < z(G_2)$.*

Proof. Let $M(G_1)$ and $M(G_2)$ be the sets of matchings of G_1 and G_2, respectively. We construct a mapping $\eta : M(G_1) \to (G_2), \forall B \in M(G_1)$

$$\eta(B) = \begin{cases} (B - \{u_r u_{r+1}\} - B \cap P^*) \cup \{u_{r+1} v_1\} \cup \xi_{P^*}(B \cap P^*), & \text{if } u_r u_{r+1} \in B \text{ and } v_1 v_2 \in B; \\ (B - \{u_r u_{r+1}\}) \cup \{u_{r+1} v_1\}, & \text{if } u_r u_{r+1} \in B \text{ and } v_1 v_2 \notin B; \\ B, & \text{otherwise} \end{cases}$$

where $P^* = u_r v_{k-1} \cdots v_2 v_1$ and ξ_{P^*} is defined in Lemma 2.3.

Note that $u_r v_{k-1} \notin B$ if $u_r u_{r+1} \in B$. The mapping η is injective. However, there is no $B \in M(G_1)$ with $\eta(B) = \{u_r u_{r-1}, u_{r+1} v_1\}$. So, $z(G_1) < z(G_2)$.

The proof is completed. $\square$

Remark 3. Repeating Transformations 1–3, any $(n, n+1)$-graph can be changed into one of the graphs $H_i(p, q)$ $(i = 1, 2, 3)$ in Fig. 5, and the Hosoya index increases by these transformations. In order to find the graph with the largest Hosoya index among all $(n, n+1)$-graphs, we only need to consider these graphs $H_i(p, q)$ in Fig. 5.

3. The largest Hosoya index of $(n, n+1)$-graphs

In this section, we first find the graph with the largest Hosoya index in $\mathcal{A}(p, q)$, and then find the graphs with the largest Hosoya indices in $\mathcal{B}(p, q)$ and in $\mathcal{C}(p, q, r)$. Finally, we compare the Hosoya indices of these graphs and characterize the extremal graphs.

Lemma 3.1. *If $n \geq 6$, $p+q = n+1$, then $z(H_1(p, q)) \leq z(H_1(4, n-3))$ with the equality if and only if $H_1(p, q) \cong H_1(4, n-3)$.*

Proof. Let $m = p = n - q + 1$. By Eq. (1), we have

$$\begin{aligned} z(H_1(p, q)) &= z(P_{m-1}) z(P_{q-1}) + 2z(P_{m-2}) z(P_{q-1}) + 2z(P_{m-1}) z(P_{q-2}) \\ &= f(m) f(q) + 2f(m-1) f(q) + 2f(m) f(q-1) \\ &= f(m) f(n-m+1) + 2f(m-1) f(n-m+1) + 2f(m) f(n-m) \end{aligned}$$

$$\begin{aligned} z(H_1(4, n-3)) &= z(P_{n-4}) z(P_3) + 2z(P_{n-5}) z(P_3) + 2z(P_{n-4}) z(P_2) \\ &= f(n-3) f(4) + 2f(n-4) f(4) + 2f(n-3) f(3) \\ &= f(n) + 4f(n-2) \\ &= f(m) f(n-m+1) + f(m-1) f(n-m) + 4f(n-2) \quad \text{(by Lemma 1.1)} \end{aligned}$$

$$\begin{aligned} z(H_1(4, n-3)) - z(H_1(p, q)) &= f(m-1) f(n-m) + 4f(n-2) - 2f(m-1) f(n-m+1) - 2f(m) f(n-m) \\ &= 2f(n-2) + 2f(n-2) + f(m-1) f(n-m) \\ &\quad - 2f(m-1) f(n-m+1) - 2f(m) f(n-m) \\ &= 2[f(m-1) f(n-m) + f(m-2) f(n-m-1) + f(m) f(n-m-1) \\ &\quad + f(m-1) f(n-m-2) - f(m-1) f(n-m+1) - f(m) f(n-m)] \\ &\quad + f(m-1) f(n-m) \quad \text{(by Lemma 1.1)} \\ &= 2[-f(m-1) f(n-m-1) + f(m-2) f(n-m-1) - f(m) f(n-m-2) \\ &\quad + f(m-1) f(n-m-2)] + f(m-1) f(n-m) \\ &= 2[-f(m-3) f(n-m-1) - f(m-2) f(n-m-2)] + f(m-1) f(n-m) \\ &= 2[-f(m-3) f(n-m-1) - f(m-2) f(n-m-2)] \\ &\quad + f(m-1) f(n-m-1) + f(m-1) f(n-m-2) \\ &= 2[-f(m-3) f(n-m-1) - f(m-2) f(n-m-2)] + f(m-2) f(n-m-1) \\ &\quad + f(m-3) f(n-m-1) + f(m-2) f(n-m-2) + f(m-3) f(n-m-2) \\ &= f(m-4) f(n-m-1) - f(m-4) f(n-m-2) \\ &= f(m-4) f(n-m-3) \geq 0 \end{aligned}$$

with the equality if and only if $m = 4$ or $m = n - 3$, i.e., $H_1(p, q) \cong H_1(4, n-3)$. $\square$

From Remark 3 and Lemma 3.1, we have immediately:

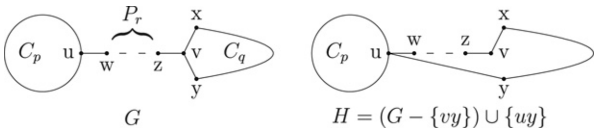

Fig. 7. The graphs in Lemma 3.3.

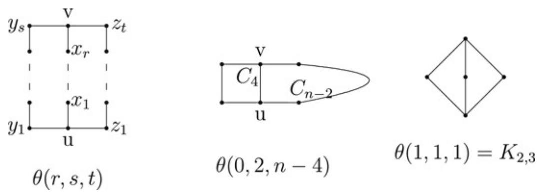

Fig. 8. The graphs in Lemma 3.5.

Theorem 3.2. *Let $G \in \mathcal{A}(p, q)$. If $n \geq 6$, then $z(G) \leq z(H_1(4, n-3))$ for all $p \geq 3$ and $q \geq 3$, with the equality if and only if $G \cong H_1(4, n-3)$.*

If $n = 5$, then $H_1(3, 3)$ is the only graph in $\mathcal{A}(p, q)$. So, the graph $H_1(3, 3)$ or $H_1(4, n-3)$ is the unique graph with the largest Hosoya index in $\mathcal{A}(p, q)$ for all $p \geq 3$ and $q \geq 3$.

Next, we show that the Hosoya indices of graphs in $\mathcal{B}(p, q)$ are less than the largest Hosoya index of graphs in $\mathcal{A}(p, q)$.

Lemma 3.3. *Let G and H be the $(n, n+1)$-graphs depicted in Fig. 7. Then $z(G) < z(H)$.*

Proof. Let $M(G)$ and $M(H)$ be the sets of matchings of G and H, respectively. We construct a mapping $\zeta : M(G) \to M(H)$, $\forall B \in M(G)$

$$\zeta(B) = \begin{cases} (B - B \cap C_q) \cup \xi_{C_q}(B \cap C_q), & \text{if } vy \in B; \\ B, & \text{otherwise} \end{cases}$$

where ξ_{C_q} is defined in Lemma 2.3 and v is taken as v_1.

Note that $vz, vx \notin B$ if $vy \in B$. The mapping ζ is injective. However, there is no $B \in M(G_1)$ with $\zeta(B) = \{uy, vx\}$. So, $z(G) < z(H)$. $\square$

From Remark 3 and Lemmas 3.1 and 3.3, we have:

Theorem 3.4. *If $G \in \mathcal{B}(p, q)$, then $z(G) < z(H_1(4, n-3))$ for all $p \geq 3$ and $q \geq 3$.*

In the following, we give the graph with the largest Hosoya index in $\mathcal{C}(p, q)$.

Lemma 3.5. *Let $\theta(r, s, t)$ and $\theta(0, 2, n-4)$ be the $(n, n+1)$-graphs depicted in Fig. 8, where $r + s + t = n - 2$. Then $z(\theta(r, s, t)) \leq z(\theta(0, 2, n-4))$, with the equality if and only if $\theta(r, s, t) \cong \theta(0, 2, n-4)$ or $\theta(r, s, t) \cong \theta(1, 1, 1)$.*

Proof. Let $G = \theta(r, s, t)$ and $H = \theta(0, 2, n-4)$. By Eq. (2), we have

$$\begin{aligned} z(G) &= z(G - \{ux_1\}) + z(G - \{u, x_1\}) \\ &= z(G - \{ux_1, vx_r\}) + z(G - \{ux_1, v, x_r\}) + z(G - \{u, x_1, vx_r\}) + z(G - \{u, x_1, v, x_r\}) \\ &= z(C_{n-r})z(P_r) + 2z(P_{r-1})z(P_{n-r-1}) + z(P_{r-2})z(P_s)z(P_t) \\ &= f(r+1)f(n-r-1) + f(r+1)f(n-r+1) + 2f(r)f(n-r) + f(r-1)f(s+1)f(t+1) \end{aligned}$$

$$\begin{aligned} z(H) &= z(H - \{uv\}) + z(H - \{u, v\}) \\ &= z(C_n) + z(P_2)z(P_{n-4}) \\ &= f(n-1) + f(n+1) + 2f(n-3). \end{aligned}$$

By Lemma 1.1,

$$\begin{aligned} f(n-r+1) &= f(s+t+3) = f(s+2)f(t+2) + f(s+1)f(t+1) \\ &> 2f(s+1)f(t+1)f(s+1)f(t+1) < \frac{1}{2}f(n-r+1). \end{aligned}$$

If $r \geq 3$, then

$$\begin{aligned}
z(H) - z(G) &= f(n+1) + f(n-1) + 2f(n-3) - f(r+1)f(n-r-1) - f(r+1)f(n-r+1) \\
&\quad - 2f(r)f(n-r) - f(r-1)f(s+1)f(t+1) \\
&= f(r+1)f(n-r+1) + f(r)f(n-r) + f(r)f(n-r) + f(r-1)f(n-r-1) \\
&\quad + 2f(r)f(n-r-2) + 2f(r-1)f(n-r-3) - f(r+1)f(n-r+1) \\
&\quad - f(r+1)f(n-r-1) - 2f(r)f(n-r) - f(r-1)f(s+1)f(t+1) \quad \text{(by Lemma 1.1)} \\
&= -f(r-2)f(n-r-1) + 2f(r)f(n-r-2) + 2f(r-1)f(n-r-3) - f(r-1)f(s+1)f(t+1) \\
&= f(r-2)f(n-r-2) + f(r-2)f(n-r-3) + 2f(r-1)f(n-r-2) \\
&\quad + 2f(r-3)f(n-r-3) - f(r-1)f(s+1)f(t+1) \\
&> \frac{1}{2}[2f(r-2)f(n-r-1) + 4f(r-1)f(n-r-2) + 4f(r-3)f(n-r-3) - f(r-1)f(n-r+1)] \\
&= \frac{1}{2}[2f(r-2)f(n-r-2) + f(r-1)f(n-r-2) + 2f(r-3)f(n-r-3)] \\
&> 0.
\end{aligned}$$

If $r = 1$, then

$$\begin{aligned}
z(H) - z(G) &= f(n+1) + f(n-1) + 2f(n-3) - f(n-2) - f(n) - 2f(n-1) \\
&= f(n-5) \geq 0
\end{aligned}$$

with the equality if and only if $n = 5$.

If $r = 2$, then $s + t = n - 4$ and

$$\begin{aligned}
z(H) - z(G) &= f(n+1) + f(n-1) + 2f(n-3) - [2f(n-3) + 2f(n-1) + 2f(n-2) + f(s+t)f(t+1)] \\
&= f(n-3) - f(s+1)f(t+1) \\
&= f(n-3) - f(s+1)f(n-s-3) \\
&= f(s)f(n-s-2) + f(s-1)f(n-s-3) - f(s+1)f(n-s-3) \quad \text{(by Lemma 1.1)} \\
&= f(s)f(n-s-4) \geq 0
\end{aligned}$$

with the equality if and only if $s = 0$ or $t = n - s - 4 = 0$. □

From Remark 3 and Lemma 3.5, we have:

Theorem 3.6. *If $G \in \mathcal{C}(p, q, r)$, then $z(G) \leq z(\theta(0, 2, n-4))$ or $z(\theta(1, 1, 1))$ for all $p \geq 3$ and $q \geq 3$, with the equality if and only if $G \cong \theta(0, 2, n-4)$ or $\theta(1, 1, 1)$.*

Now, in order to find the graph with the largest Hosoya index among all $(n, n+1)$-graphs, we only need to compare the Hosoya indices of $H_1(3, 3)$, $H_1(4, n-3)$, $\theta(0, 2, n-4)$ and $\theta(1, 1, 1)$.

$z(H_1(3, 3)) = 12$, $\quad z(\theta(1, 1, 1)) = z(\theta(0, 2, 1)) = 13$.

From the proofs of Lemmas 3.1 and 3.5, we know that

$$z(H_1(4, n-3)) = f(n) + 4f(n-2), \qquad z(\theta(0, 2, n-4)) = f(n+1) + f(n-1) + 2f(n-3).$$

Thus $z(\theta(0, 2, n-4)) - z(H_1(4, n-3)) = 2f(n-5)$. So, we have:

Main Theorem. If $n \geq 6$, then $\theta(0, 2, n-4)$ is the unique graph with the largest Hosoya index among all $(n, n+1)$-graphs. If $n = 5$, then $\theta(0, 2, 1)$ and $\theta(1, 1, 1)$ are the graphs with the largest Hosoya index of all (5,6)-graphs.

For $n = 4$, it is trivial since there is exactly one (4,5)-graph.

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